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Use of Kriging to Estimate Monthly Ozone Exposure Parameters for the Southeastern United States (Journal Version)

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16. ABSTRACT

This paper explores the feasibility of (1) using kriging to predict the monthly mean of daily 7-h mean (0900-1559) O_3 concentrations, (2) using kriging to estimate the percent of hourly mean O_3 concentrations equal to or greater than 0.07 ppm (137 μg m^{-3}) for a specific month, and (3) developing a quantitative relationship between the monthly mean of the daily 7-h (0900-1559) average O_3 concentration and the monthly number of hourly concentrations ≥0.08 ppm (157 μg m^{-3}). We found that kriging can be used to estimate the (1) monthly mean of daily 7-h mean O_3 concentrations and (2) the percentage of hourly concentrations for a given month ≥0.07 ppm when sufficient spatial coverage was available. However, the percent ≥0.07 ppm parameter exhibited much greater relative variability than the monthly 7-h exposure index. A strong statistical association was found between the monthly number of occurrences ≥0.08 ppm and monthly 7-h mean concentrations above 0.05 ppm (98 μg m^{-3}). Because of the variability that cumulative indices, such as the monthly percentage of hourly concentrations ≥0.07 ppm, exhibit from site to site, it appears that whether kriging techniques or mathematical regressions are used to estimate the number of elevated O_3 hourly concentrations above selected thresholds, large uncertainties associated with the predicted values will exist. These large uncertainties will make it difficult to accurately estimate vegetation effects caused by ambient levels of O_3. However, if a generalized quantitative relationship between repeated occurrences of hourly mean concentrations ≥0.07 or ≥0.08 ppm and vegetation effects can be developed, it may be possible, using kriged monthly values accompanied with confidence intervals, to identify those areas where vegetation may be at risk. However, before it will be possible to implement such an approach, researchers will have to better quantify the relationship between realistic O_3 exposures and vegetation effects.

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The Use of Kriging to Estimate Monthly Ozone Exposure Parameters for the Southeastern United States

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ABSTRACT

This paper explores the feasibility of (1) using kriging to predict the monthly mean of daily 7-h mean (0900-1559) O_3 concentrations, (2) using kriging to estimate the per cent of hourly mean O_3 concentrations equal to or greater than 0·07 ppm (137 $\mu g\,m^{-3}$) for a specific month, and (3) developing a quantitative relationship between the monthly mean of the daily 7-h (0900-1559) average O_3 concentration and the monthly number of hourly concentrations ≥0·08 ppm (157 $\mu g\,m^{-3}$). We found that kriging can be used to estimate the (1) monthly mean of daily 7-h mean O_3 concentrations and (2) the percentage of hourly concentrations for a given month ≥0·07 ppm when sufficient spatial coverage was available. However, the per cent ≥0·07 ppm parameter exhibited much greater relative variability than the monthly 7-h exposure index. A strong statistical association was found between the monthly number of occurrences ≥0·08 ppm and monthly 7-h mean concentrations above 0·05 ppm (98 $\mu g\,m^{-3}$). Because of the variability that cumulative indices, such as the monthly percentage of hourly concentrations ≥0·07 ppm, exhibit from site to site, it appears that whether kriging techniques or mathematical regressions are used to estimate the number of elevated O_3 hourly concentrations above selected thresholds, large uncertainties associated with the predicted values will exist. These large uncertainties will make it difficult to accurately estimate vegetation effects caused by ambient levels of O_3. However, if a generalized quantitative relationship between repeated occurrences of hourly mean concentrations ≥0·07 or ≥0·08 ppm and vegetation effects can be developed, it may be possible, using kriged monthly values accompanied with confidence intervals, to identify those areas where vegetation may be at risk. However, before it will be possible to implement such an approach, researchers will have to better quantify the relationship between realistic O_3 exposures and vegetation effects.

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INTRODUCTION

Kriging has been used to estimate O_3 levels across the United States. The National Crop Loss Assessment Network (NCLAN) used kriging to estimate 5-month seasonal mean O_3 levels to predict the effects of O_3 on vegetation (Heck *et al.*, 1984). To provide better time resolution for estimating O_3 levels, Lefohn & Knudsen (1987*a*) explored the use of kriging to predict monthly means of the daily means of the maximum 7- and 12-h O_3 concentrations for 68 regions across the United States. Lefohn & Knudsen (1987*b*) further extended this work to the southeastern United States, using all available 1984 O_3 7-h (0900–1559) monthly data from O_3 sites to krig monthly data by $0.5^\circ \times 0.5^\circ$ grids.

Most of the research associated with using kriging to predict O_3 concentrations has focused on estimating seasonal and monthly 7-h values. However, the US Environmental Protection Agency (1986) and Lefohn & Runeckles (1987) have discussed the importance of O_3 peak concentrations in eliciting injury and yield reduction for agricultural crops. Therefore, kriging, used for predicting monthly O_3 exposure information, is of potential importance to those scientists who desire to estimate exposure indices that describe the occurrences of elevated O_3 concentrations. Examples of indices that might be helpful in describing elevated O_3 concentrations are the percentage or number of hourly occurrences equal to or above selected threshold concentrations. Lefohn *et al.* (1988) have described the use of several exposure indices that emphasize elevated hourly O_3 concentrations for assessing possible O_3 effects on agricultural crops.

Two approaches that might be useful for estimating exposure indices that characterize elevated hourly O_3 concentrations are: (1) using kriging to predict the per cent of occurrences $\geq$ a selected minimum concentration and (2) using kriging to predict the monthly mean of the 7-h concentrations and then regressing this exposure index against the number of hourly occurrences $\geq$ a selected threshold. This paper focuses on the two suggested approaches.

For assessing the efficacy of the two approaches, data reported in previous studies using sites in the southeastern United States (Lefohn & Knudsen 1987*b*,*c*) were used to explore (1) the use of kriging to predict the monthly mean of daily 7-h mean O_3 concentrations and (2) the use of kriging to estimate directly the per cent of hourly mean O_3 concentrations ≥ 0.07 ppm for a specific month. In addition (1) the strength of the association between the monthly mean of daily 7-h (0900–1559) average concentrations and the monthly number of hourly concentrations ≥ 0.08 ppm ($157\ \mu g\ m^{-3}$) and (2) the prediction of the number of occurrences ≥ 0.08 ppm from kriged monthly means of the daily 7-h average concentrations were investigated.

While it might have been beneficial for the investigation to use consistent cumulative exposure indices (e.g. either per cent ≥ 0.07 ppm or number of occurrences ≥ 0.08 ppm) throughout the analyses, the investigators were constrained by the characterized O_3 data that were available from the Southern Forest Atlas Project of the National Vegetation Survey within the joint US Environmental Protection Agency—USDA Forest Service Forest Response Program. Because of the strong association between the monthly per cent of hourly concentrations ≥ 0.07 ppm and the number of occurrences of hourly concentrations ≥ 0.08 ppm that would be expected to occur during a given month, the results obtained would be anticipated to be similar to those obtained if a set of consistent cumulative indices had been used throughout the analyses.

METHOD

Hourly mean concentration information from the US Environmental Protection Agency's (EPA) SAROAD database was used to calculate monthly 7-h (0900–1559) O_3 values for the months April to October for 1983 and 1984. A monthly mean for a specific monitoring site was used only if $\geq 75\%$ of the hourly O_3 concentrations were available for a given month. Data surrounding and within the southeastern United States (Alabama, Arkansas, Florida, Georgia, Kentucky, Louisiana, Mississippi, North Carolina, Oklahoma, South Carolina, Tennessee, Texas, and Virginia) were used.

For kriging the per cent of hourly occurrences ≥ 0.07 ppm for a specific month, data from the EPA SAROAD database, augmented by the Tennessee Valley Authority and National Park Service databases, were used. Only monitoring sites in the southeastern United States having $\geq 50\%$ capture in any given month were used. For this part of the study, only data for May and July 1983 were incorporated in the analysis.

To explore the statistical relationship between the monthly means of the daily 7-h (0900–1559) and monthly number of hourly concentrations ≥ 0.08 ppm, data from the EPA SAROAD database, augmented by the EPRI-SURE/-ERAQS, Tennessee Valley Authority, and National Park Service databases were used. The data were compiled from 1978 through 1984 readings. Only those sites with $\geq 70\%$ data capture per given month were included in the analysis. The data used were limited to those collected at forested and agricultural sites located in the southeastern United States. Monitoring sites which were located in areas $\geq 50\%$ forested were designated as 'forested'. Those monitoring sites that were located in areas $\geq 50\%$ agricultural were considered 'agricultural'. Aerial photographs

obtained by the US Forest Service and the Forest Insect and Disease Management Aerial Survey Team in Doraville, Georgia, were interpreted by the Forest Service to identify sites located in agricultural and forested areas. The Pearson's correlation coefficient was used to quantify the statistical association between monthly (1) mean 7-h concentrations and (2) number of hourly concentrations $\geq 0{\cdot}08$ ppm.

In its original 1982 analysis (Heck *et al.*, 1984), NCLAN was concerned that O_3 concentrations may be lower at center-city than at rural locations; specific monitoring stations located in large metropolitan areas were not included. The 'filtering' protocol originally implemented by NCLAN to reduce the bias associated with using center-city monitoring sites was also applied in our analysis; selected center-city sites near metropolitan areas were removed.

Before using ordinary kriging to predict the monthly 7-h (0900–1559) O_3 concentration for $0{\cdot}5° \times 0{\cdot}5°$ grids in the southeastern United States, the O_3 data were inspected to verify that they were spatially correlated, displayed an approximately constant variance across the region being studied, and exhibited little or no drift. The 'leave one out' technique (Knudsen & Kim, 1979) was used to validate the variogram models. In this technique, the surrounding sites, but not the site being predicted, were used to predict the O_3 concentration at a monitoring site. The predicted value was then compared to the known O_3 value for that site. When all sites had been predicted in this way, the statistics of the prediction errors were computed. If the variogram behaved properly, the prediction errors were expected to have a mean of zero and variance equal to the kriging variance that is calculated from the variogram. The same procedure was used to verify the variograms used to predict the per cent of hourly occurrences $\geq 0{\cdot}07$ ppm.

RESULTS

Estimating monthly 7-h means for the Southeastern United States

The mean of the daily 7-h means (0900–1559) was estimated for the months April through October for 1983 and 1984. Only the results for July 1984 are discussed. Figure 1 illustrates O_3 monitoring sites used for estimating the July 1984 values.

The omnidirectional variogram obtained from the July data is shown in Fig. 2. Overall the variograms obtained for each month were consistent in the degree of spatial continuity exhibited, but the variance of the data is lower in the spring and fall than in the summer. As in previous studies for the

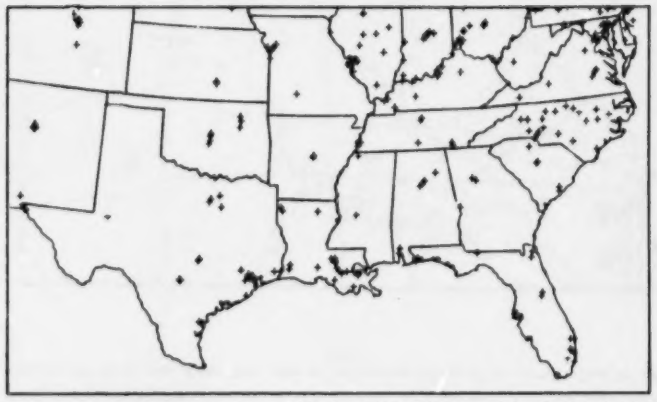

Fig. 1. Sites used to estimate the monthly 7-h (0900–1559) mean value for July 1984.

entire United States (Lefohn *et al.*, 1987), the variograms were found to be anisotropic. Statistical results of the variogram validation are shown in Table 1. The variance of observed errors is very close to the predicted kriging variance, indicating that the variogram model used was appropriate.

The results of kriging the monthly 7-h mean values are shown in Fig. 3. The 95% error bounds for the monthly 7-h means are shown in Fig. 4. The relative error bound for any $0{\cdot}5° \times 0{\cdot}5°$ cell is approximately plus or minus 20% of the kriged value.

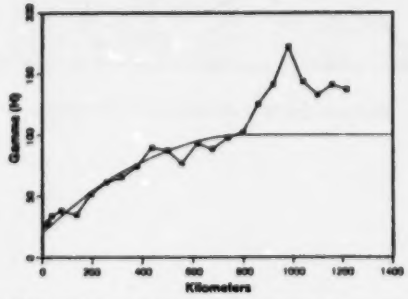

Fig. 2. The July 1984 omni-directional variogram calculated from monthly 7-h values.

TABLE I

Summary Statistics of Kriging Errors Using Leave-one-out Validation Analysis for the 7-h Ozone Variable. The Mean Value is Expressed in Units of ppm, and the Variance is Expressed in ppm Squared

July 1984 Validation	
Mean	0·000 25
Variance	0·000 035 6
Std. Deviation	0·000 005 96
Avg. Krig Variance	0·000 034 6
Pct. of Errors within Two Std. Deviations	96·20

Estimating the per cent of occurrences of hourly mean concentrations ≥0·07 ppm

Information from approximately 150 sites was available with better than 50% data capture for the May and July 1983 periods. The location of the sites and their values for July 1983 are shown in Fig. 5.

For the actual data used in the kriging analysis, the per cent of occurrences of hourly mean concentrations ≥0·07 ppm has a greater relative variability than the monthly mean 7-h parameter. For May 1983, the variable had a

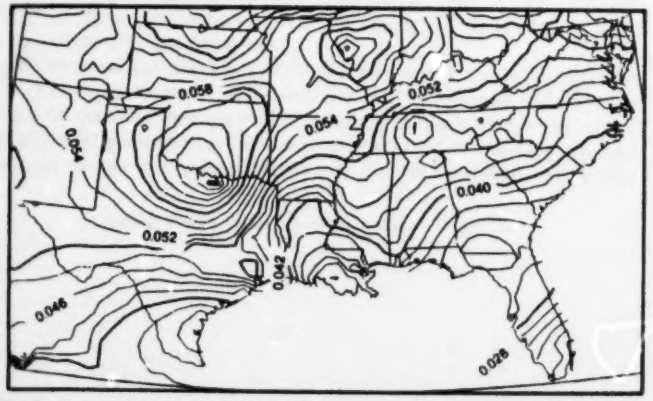

Fig. 3. Contour plot of the kriged estimates (concentrations in ppm) of the monthly 7-h (0900–1559) mean value for July 1984.

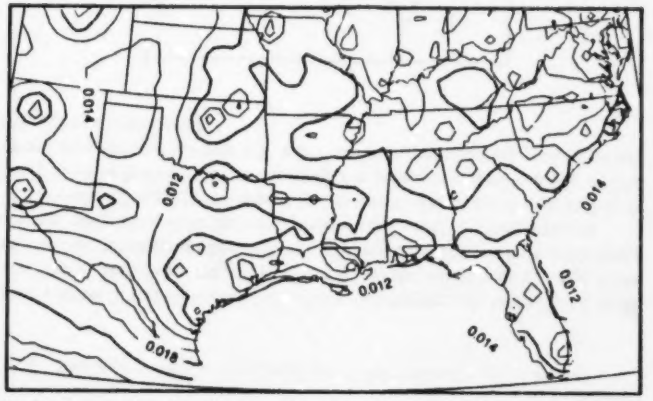

Fig. 4. Contour plot of the 95% error bound for the estimated 7-h mean values for July 1984.

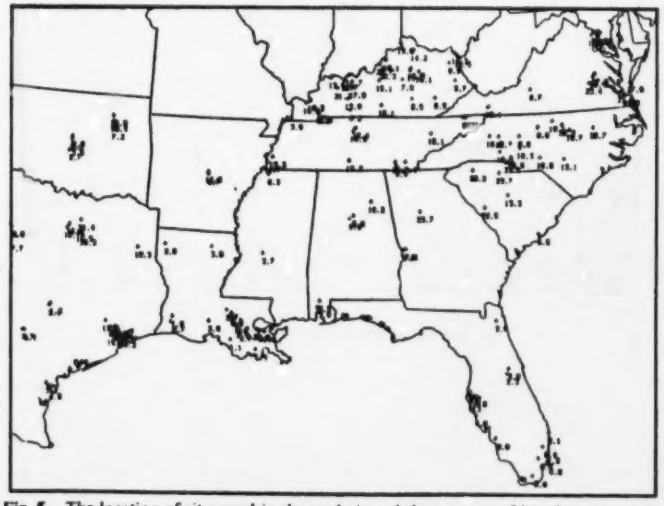

Fig. 5. The location of sites used in the analysis and the per cent of hourly occurrences ≥0·07 ppm for July 1983.

coefficient of variation (CV) of 1·07, while the 7-h mean had a CV of 0·20. The corresponding numbers for July 1983 were 0·66 and 0·25. The per cent of occurrences of hourly mean concentrations variables had a strong positive skewness (1·62 and 0·35 in May and July, respectively), whereas the monthly mean 7-h values were nearly symmetric. A scatter plot of the variable versus the monthly 7-h parameter is shown in Fig. 6. The plot shows a definite relationship between the monthly mean 7-h value and the per cent of hourly occurrences ≥0·07 ppm. Over the entire range of values, the relationship is not linear; however, for the 7-h monthly values > approximately 0·05 ppm, a more linear relationship emerges.

Because of the high relative variability of the per cent of hourly occurrences ≥0·07 ppm variable, the variograms calculated were not as smooth as the mean 7-h variograms. Omnidirectional variograms for May and July are shown in Fig. 7. Both variograms show fairly large fluctuations of the variogram values. These variograms show that the variable is spatially correlated and that the limit of this correlation is about 1500 km. For interpolation purposes, data 900 km from the point or area being estimated were not used in the analysis. Spherical variogram models were fitted to the omnidirectional variograms and are shown as the smooth solid lines on each variogram. Directional variograms were calculated, but the fluctuations were too large to determine if anisotropy existed.

Statistical results of the validations for May and July 1983 are shown in Table 2. In the May model, the variance of errors is nearly identical to the predicted kriging variance, and the mean error is almost zero. In the July model, the observed variance of errors is about 12% larger than the kriging

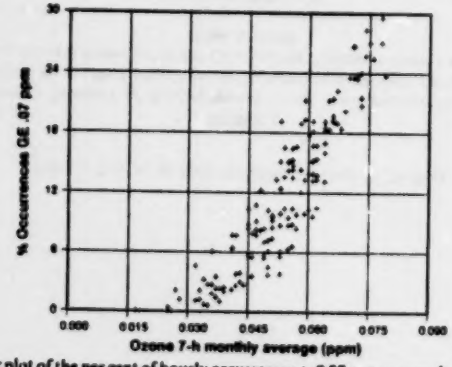

Fig. 6. Scatter plot of the per cent of hourly occurrences ≥0·07 ppm versus the monthly 7-h values for July 1983.

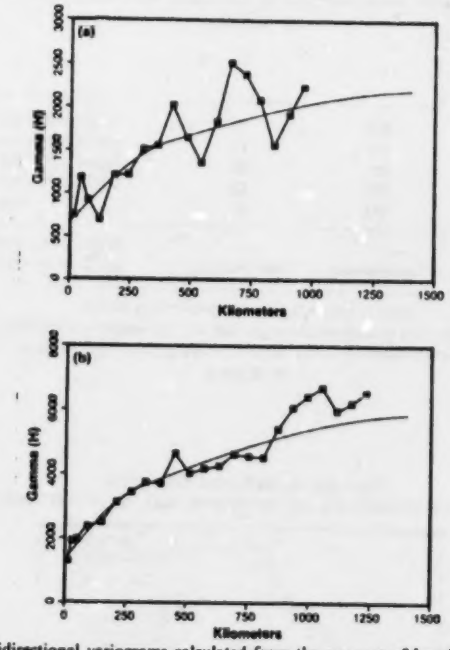

Fig. 7. Omnidirectional variograms calculated from the per cent of hourly occurrences ≥0·07 ppm for (a) May 1983 and (b) July 1983.

variance. Examination of the site-by-site results showed that a few adjacent sites with widely differing values contributed most of the variance. Such results are not unexpected when the data are highly skewed and have a high CV.

Ordinary kriging was used to estimate the monthly per cent of hours ≥0·07 ppm by 0·5° by 0·5° grids for May and July for North Carolina, South Carolina, and Geoergia. The kriging results for July 1983 are shown in Fig. 8. The 95% error bounds on the kriging results are shown in Fig. 9. The relative error bound for a cell varies from about ±50% to almost ±100%.

Association between 7-h means and number of occurrences ≥0·08 ppm

The correlation coefficients between 7-h means and number of hourly occurrences ≥0·08 ppm were 0·770 and 0·741 when sites characterized as

TABLE 2

Summary Statistics of Kriging Errors Using Leave-one-out Validation Analysis for the Per Cent of Hourly Occurrences ≥0·07 ppm Variable. The Mean Value is Expressed in Per Cent and the Variance is Expressed in Per Cent Squared

May 1983 Validation	
Mean	0·01
Variance	9·26
Std. Deviation	3·04
No. of Sites	138
Avg. Krig Variance	9·52
Pct. of Errors Within Two Std. Deviations	93·48
July 1983 Validation	
Mean	0·12
Variance	23·94
Std. Deviation	4·88
No. of Sites	139
Avg. Krig Variance	21·31
Pct. of Errors Within Two Std. Deviations	94·96

forested and agricultural, respectively, were used (Tables 3a and 3b). Though the forest and agriculture data subsets demonstrated slightly different results, the strength of the association between the two variables showed a clear tendency to increase as sites with low 7-h monthly values were deleted from the database (Tables 3a and 3b). Such a tendency indicates the paucity of hourly mean concentrations ≥0·08 ppm for those sites where low monthly 7-h mean O_3 concentrations were experienced. For example, Tables 3a and 3b show low correlation coefficients when the database is restricted solely to 7-h monthly mean values ≤0·05 ppm (98 $\mu g\,m^{-3}$) and ≤0·04 ppm (78 $\mu g\,m^{-3}$).

Fig. 8. Contour plot of the kriged estimates of the per cent of hourly occurrences ≥0·07 ppm for July 1983.

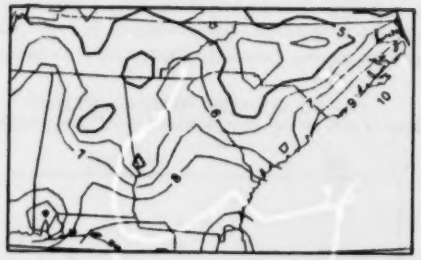

Fig. 9. Contour plot of the 95% error bound for the estimated per cent of hourly occurrences ≥0·07 ppm for July 1983.

TABLE 3a

Correlation Coefficients Between 7-h Monthly Mean Ozone Concentrations and the Number of Monthly Occurrences ≥0·08 ppm for Selected Forested Sites in the Southeastern United States. Concentrations are Expressed in ppm

Specified range of 7-h monthly mean values	*Different sites*	*Site-months*	*Corr. coefficient*
all data	31	530	0·770
all 7-h values > 0·05	27	162	0·796
all 7-h values > 0·06	18	54	0·743
all 7-h values ≤ 0·05	31	368	0·519
all 7-h values ≤ 0·04	28	219	0·378

TABLE 3b

Correlation Coefficients Between 7-h Monthly Mean Ozone Concentrations and the Number of Monthly Occurrences ≥0·08 ppm for Selected Agricultural Sites in the Southeastern United States. Concentrations are expressed in ppm

Specified range of 7-h monthly mean values	*Different sites*	*Site-months*	*Corr. coefficient*
all data	34	937	0·741
all 7-h values > 0·05	31	256	0·825
all 7-h values > 0·06	24	82	0·817
all 7-h values ≤ 0·05	34	681	0·528
all 7-h values ≤ 0·04	32	448	0·323

TABLE 4

Statistical Summary of Differences Between the Estimated Minus Actual Values when Regression Equations are Used to Predict the Number of Monthly Hourly Occurrences ≥0·08 when 7-h Monthly Mean Concentrations >0·05 ppm are Used. The Mean Value is Expressed in Units of ppm, and the Variance is Expressed in ppm Squared

	Agricultural	*Forested*
Mean	0·00	0·00
Variance	0·000 279 77	0·000 354 73
Std. Deviation	0·016 72	0·018 83
No. of Site-Months	256	162

The forested subset of data experienced the highest correlation coefficients when monthly 7-h values >0·05 ppm were used. For the agricultural data subset, the highest correlation coefficients occurred when monthly 7-h values exceeding 0·05 ppm were used.

Using the monthly data with 7-h concentrations >0·05 ppm, the following linear regression equations were obtained relating the monthly 7-h values with number of hourly mean concentrations ≥0·08 ppm;

Agricultural: $Y = -202 + 4199 \times 7\,h$

Forested: $Y = -158 + 3417 \times 7\,h$

where Y is the number of hourly mean O_3 concentrations ≥0·08 ppm and 7 h is the monthly mean of the daily 7-h (0900–1559) O_3 concentrations for 7-h values >0·05 ppm. The estimated value for the number of hourly mean concentrations ≥0·08 ppm was calculated for each site-month of data and compared with the actual value. The variance was large for both the agricultural and forested sites (Table 4).

DISCUSSION

Kriging can be used to estimate the (1) 7-h monthly means and (2) monthly percentage of hourly means ≥0·07 ppm when sufficient spatial coverage is available. However, kriging should not be used to predict O_3 exposures at high elevation locations unless sufficient spatial coverage is available. Some high elevation sites exhibit O_3 exposure characteristics that are distinct from those observed at lower elevation sites (Berry, 1964; Stasiuk & Coffey, 1974; Mohnen *et al.*, 1977; Miller *et al.*, 1986; Lefohn & Jones, 1986; Lefohn & Mohnen, 1986). The differences in O_3 exposure patterns will make it difficult

to adequately predict exposures experienced at high elevation sites using data from lower elevation areas.

In our analysis, we found that the kriged estimates of the per cent of hours ≥0·07 ppm had a much larger relative prediction error variance (i.e. kriging variance) than the kriged estimates of the monthly 7-h means. The larger kriging variance is due to the high variability inherent in the observed data values of the per cent of hours ≥0·07 ppm. The monthly 7-h value changes more slowly from site to site than the per cent ≥0·07 ppm parameter and thus provides a kriged estimate that exhibits smaller deviations from the actual value. Because the monthly 7-h value is an average compiled from the mean of seven consecutive hourly values, the monthly 7-h value does not vary over a large magnitude. The per cent ≥0·07 ppm parameter, on the other hand, is a cumulative index and is more susceptible to variability induced by the occurrences of a few high hourly concentrations, which affect the monthly 7-h mean only marginally. The magnitude of the kriging variance and resulting uncertainty in the estimates of the per cent of hourly mean concentrations ≥0·07 ppm parameter may limit the usefulness of the kriged estimates.

Lefohn & Benedict (1985) discussed the shortcomings associated with relating seasonal average concentrations (e.g. the daily means of 7- and 12-h O_3 concentrations over a multiple-month period) with exposure indices that focus on episodic O_3 exposures (e.g. cumulative indices). However, we have found that strong statistical associations exist between the two types of indices over a shorter time period (i.e. a month) when monthly 7-h concentrations ≥0·05 ppm were used. The correlation coefficient decreased when only low 7-h monthly values were used; when 7-h monthly values ≤0·05 ppm were used, the coefficient was only 0·519 (Table 3). If monthly 7-h values at a particular site tend to be <0·05 ppm, one would expect a relatively weak association between the monthly 7-h average and the number of occurrences >0·08 ppm. For sites with monthly 7-h values in the 0·05 to 0·06 ppm (98 to 118 $\mu g\,m^{-3}$) range, the association between the monthly 7-h and the number of occurrences ≥0·08 ppm would be expected to be stronger.

The strong statistical association described above implies that a model might be constructed that mathematically could estimate values for selected cumulative indices when 7-h mean values were determined. However, it should be noted that any resulting estimate would have two sources of error. First, the monthly 7-h kriged mean value does have an error associated with its estimate; and, secondly, uncertainties are associated with the application of any regression model. Because of the variability that cumulative indices, such as the monthly percentage of hourly concentrations ≥0·07 ppm or number of hourly concentrations ≥0·08 ppm, exhibit from site to site, it

appears that whether kriging techniques or mathematical regressions are used to estimate the number of elevated O_3 hourly concentrations above selected thresholds, large uncertainties associated with the predicted values will exist.

The US Environmental Protection Agency (1986) and Lefohn & Runeckles (1987) have discussed the shortcomings associated with using long-term mean exposure indices, such as the 7-h seasonal mean, for predicting vegetation effects and have recommended that additional attention be given to the higher concentrations while still including the lower hourly concentrations in describing exposures. The large uncertainties associated with using kriging to predict values for cumulative indices that summarize elevated exposures will make it difficult to accurately estimate vegetation effects caused by ambient levels of O_3. However, should repeated occurrences of hourly mean concentrations $\geq 0{\cdot}07$ or $\geq 0{\cdot}08$ ppm be found to elicit adverse vegetation effects, then, using kriged monthly values accompanied with confidence intervals, it may be possible to identify those areas where vegetation may be at risk. However, before it will be possible to implement such an approach, researchers will have to better quantify the relationship between realistic O_3 exposures and vegetation effects.

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